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FINAL TECHNICAL REPORT

U.S. OFFICE OF NAVAL RESEARCH GRANT N00014-90-J-1871

Investigations of Non-elliptic Elastic Materials and the Modeling of Phase Transformations in Solids

This grant to the California Institute of Technology covered the period May 1, 1990 - April 30, 1993. It has included a subcontract to the Massachusetts Institute of Technology to facilitate collaboration between Professors R. Abeyaratne of M.I.T. and J.K. Knowles of Caltech. During the period covered by this grant and its predecessor, the collaborators and their Ph.D. students have studied the modeling of displacive phase transitions in solids in a continuum mechanical framework. The six most fundamental accomplishments of this work are as follows.

(i) We have shown that the fully nonlinear theories of elasticity and thermoelasticity, which describe materials that are free of internal dissipation, are nevertheless capable of modeling the hysteretic behavior associated with displacive phase transitions, provided the underlying elastic potential or Helmholtz free energy is "non-elliptic" and phase boundaries are modeled as moving surfaces of strain discontinuity.

(ii) Through energy and entropy considerations within the theory of moving strain discontinuities in a continuum, we have identified a general notion of "driving traction" acting on a phase boundary. The driving traction is an agent of dissipation associated with interfaces between phases and, in the case of slow processes, it is identical with the materials scientists' concept of driving force as the jump in Gibbs free energy across a phase boundary. This notion has turned out to be of fundamental importance.

(iii) We have shown that the basic balance principles of continuum mechanics and the elastic (or thermoelastic) constitutive law are not by themselves capable of rendering the theory of elastic or thermoelastic materials fully determinate when such materials are capable of undergoing phase transitions; additional constitutive information is required. In our modeling, we remedied this constitutive deficiency by imposing a "nucleation criterion" and a "kinetic relation" between the driving traction and the velocity of the phase boundary. We have thus been able to import these two important concepts from materials science into the continuum mechanical model of the macroscopic behavior of solids capable of undergoing displacive phase transitions.

(iv) In a purely mechanical setting, we have shown that the kinetic relation and the nucleation criterion can be accommodated in the continuum *dynamics* of phase transitions, and that notions of *admissibility* of rapidly propagating phase boundaries introduced earlier by others can be subsumed under our theory by choosing an appropriate kinetic relation.

(v) We have tested these fundamental ideas in two ways: (1) by solving specific analytical problems in quasi-statics and in dynamics in both purely mechanical and thermomechanical settings in order to be certain that the theory can in fact be used to solve problems, and (2) by comparing qualitatively the predictions of the theory with experimental observations.

(vi) Five graduate students (E. Fried, Q. Jiang, M. Lusk, and P. Rosakis of Caltech and G.-H. Jiang of M.I.T.) have received Ph.D. degrees after successfully defending dissertations based on research carried out under this grant or under its predecessor. Two more (Y. Lin of M.I.T., J. Restuccio of Caltech) are nearly finished.

In work carried out under the predecessor of this grant, we began our investigation of non-elliptic elastic materials with fundamental studies of stress-induced equilibrium mixtures of phases - or quasi-static motions involving such mixtures - in a purely mechanical setting that was based on finite elasticity and that ignored thermal effects; see, for example, the papers [1-3] in the list of references at the end of this report. Still in the purely mechanical context, we next showed that the incorporation of notions of nucleation and kinetics into the theory led to predictions that were in qualitative accord with experimental observations involving slowly propagating phase boundaries; see [4]. Next, we demonstrated that the notion of driving traction identified in this limited context had meaning and significance in *any* deforming continuum, regardless of its constitutive law, even when inertial and thermal effects were taken into account [5]. Still in the purely mechanical framework, we proved that there was room in the *dynamical* theory of nonlinear elasticity for the nucleation criterion and the kinetic relation, and that other approaches to the continuum dynamics of phase transitions could be subsumed under our theory [6-8].

Along the way, we have investigated the quality of a geometrically linear, physically nonlinear version of the theory as applied to the reduction of stress concentration (G.-H. Jiang [9, 10]), we have applied a thermoelastic model to the interpretation of results of a laboratory experiment of interest in geophysics (Q. Jiang [11]), we have studied the stability of elastic or thermoelastic phase boundaries (Fried [12, 13]), we have generalized the model to account for the effects of "interfacial structure" of phase boundaries that materials scientists consider to be important (Lusk [14]). Detailed studies are underway involving one-dimensional dynamical problems in the purely mechanical theory (Lin) and the incorporation of the effects of anisotropy (Restuccio).

The most recent investigations under this grant are those reported in papers [15-17]. In the first of these, we show that a material capable of undergoing phase transitions can be exploited to control the reflection or transmission of a wave that is incident upon it. The distinction in

dynamics between elastic materials that are capable of phase-transformation and those that are not is studied in [16]. In [17], we give a simple one-dimensional thermoelastic model for phase transitions, including a Helmholtz free energy, a thermally activated kinetic relation and an explicit nucleation criterion, and we carry out an extensive qualitative comparison of the predictions of this model in quasi-statics with experimental results from the materials science literature.

As to the future, our most immediate objective is to explore the predictions of the one-dimensional thermoelastic model mentioned above in a *dynamical* problem corresponding to fast phase transitions. In the longer term, we wish to study problems in two or three dimensions; such problems offer challenges not present in the one-dimensional models that have formed the basis for much, though not all, of our work up to now.

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